

## Supporting Information

### Systematic study of the luminescent europium-based nonanuclear clusters with modified 2-hydroxybenzophenone ligands

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Table S1. Crystal data and details of data collection and refinement

Compound reference	Eu9-1	Eu9-2	Eu9-3	Eu9-4	Eu9-6
Chemical formula	C <sub>146</sub> H <sub>165</sub> Eu <sub>9</sub> O <sub>62</sub>	C <sub>208</sub> H <sub>153</sub> Eu <sub>9</sub> O <sub>42</sub>	C <sub>224</sub> H <sub>185</sub> Eu <sub>9</sub> O <sub>58</sub>	C <sub>240</sub> H <sub>217</sub> Eu <sub>9</sub> O <sub>58</sub>	C <sub>224</sub> H <sub>169</sub> Eu <sub>9</sub> F <sub>16</sub> O <sub>42</sub>
Formula Mass	4279.51	4692.09	5172.51	5396.93	5204.36
Crystal system	monoclinic	triclinic	monoclinic	tetragonal	tetragonal
<i>a</i> /Å	22.8555(5)	18.5229(2)	27.2191(5)	19.265(3)	26.3718(3)
<i>b</i> /Å	26.3764(6)	18.6089(2)	28.5350(4)	19.265(3)	26.3718(3)
<i>c</i> /Å	31.4562(7)	32.1233(4)	36.3189(6)	31.373(6)	36.6258(6)
$\alpha$ /°	90.00	86.8477(9)	90.00	90.00	90.00
$\beta$ /°	101.610(2)	81.2567(10)	107.0859(18)	90.00	90.00
$\gamma$ /°	90.00	87.2640(10)	90.00	90.00	90.00
Unit cell volume/Å <sup>3</sup>	18575.2(7)	10918.7(2)	26963.8(7)	11644(3)	25472.3(6)
Temperature/K	291(2)	291(2)	291(2)	291(2)	291(2)
Space group	<i>P</i> 21/ <i>c</i>	<i>P</i> -1	<i>C</i> 2/ <i>c</i>	<i>I</i> 422	<i>P</i> 41212
<i>Z</i>	4	2	4	2	4
Radiation type	Mo K $\alpha$	Mo K $\alpha$	Mo K $\alpha$	MoK $\alpha$	MoK $\alpha$
Absorption coefficient, $\mu$ /mm <sup>-1</sup>	3.066		2.124	2.463	2.253
No. of reflections measured	85972		68745	13113	57771
No. of independent reflections	37843		26710	5960	25812
<i>R</i> <sub>int</sub>	0.0324		0.0387	0.0569	0.0487
Final <i>R</i> <sub>i</sub> values ( <i>I</i> > 2 $\sigma$ ( <i>I</i> ))	0.0392		0.0356	0.0441	0.0414
Final <i>wR</i> ( <i>F</i> <sup>2</sup> ) values ( <i>I</i> > 2 $\sigma$ ( <i>I</i> ))	0.0981		0.0953	0.0851	0.0805
Final <i>R</i> <sub>i</sub> values (all data)	0.0590		0.0549	0.0643	0.0608
Final <i>wR</i> ( <i>F</i> <sup>2</sup> ) values (all data)	0.1067		0.1017	0.0933	0.0875
Goodness of fit on <i>F</i> <sup>2</sup>	0.994		0.996	0.998	1.034

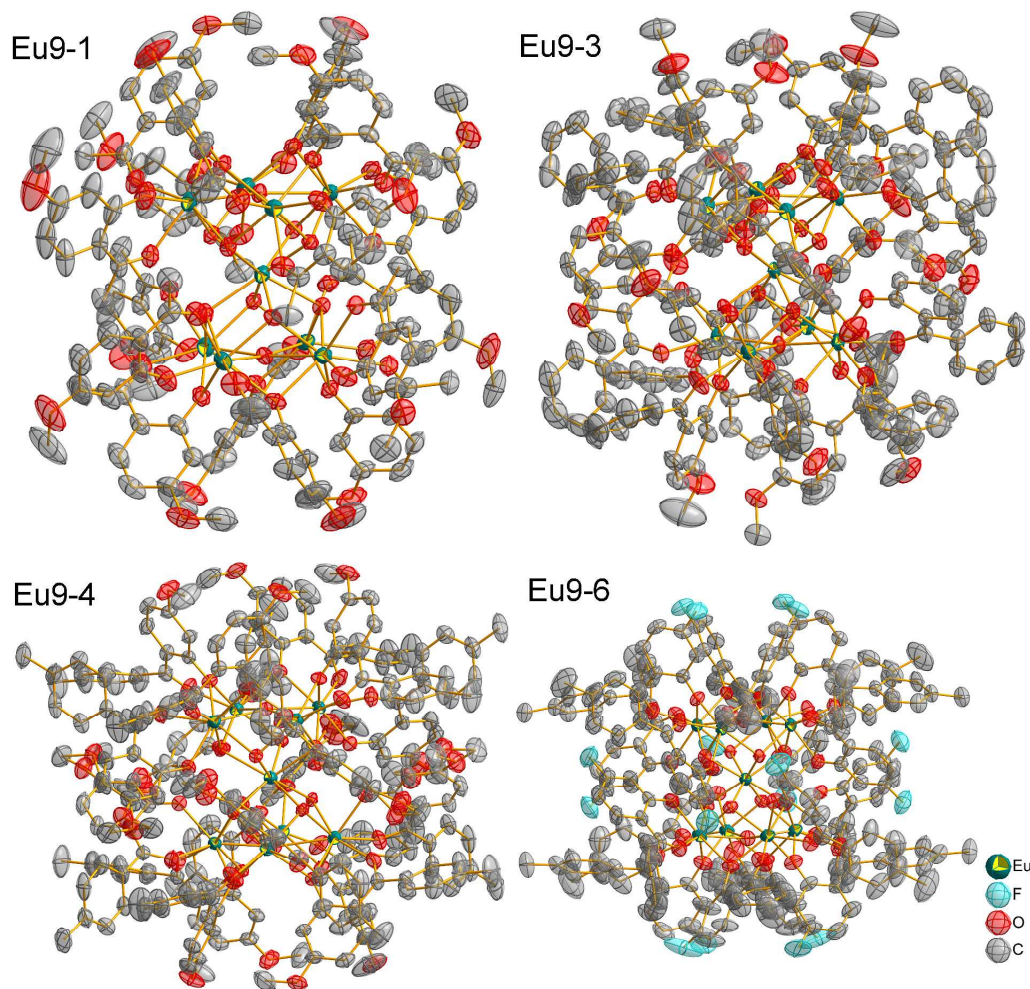


Figure S1. ORTEP diagram of the clusters with thermal ellipsoids drawn at the 50% probability level. For clarity, hydrogen atoms have been omitted.

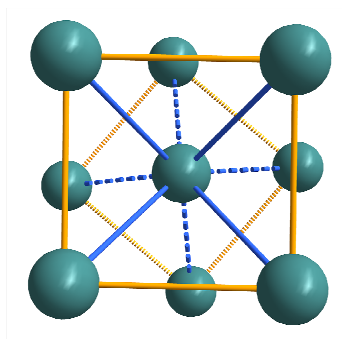
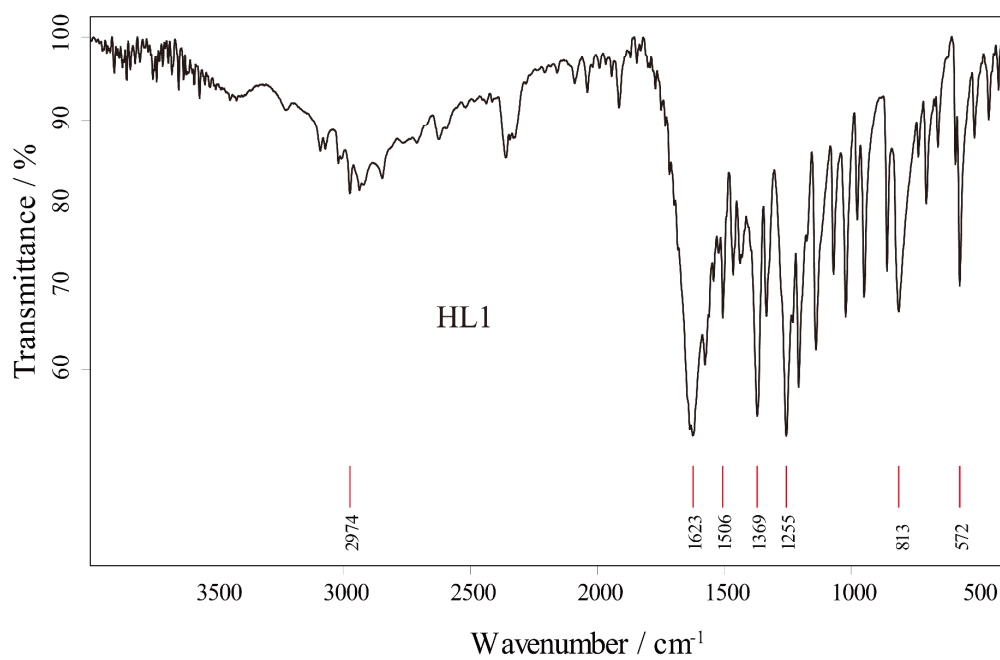
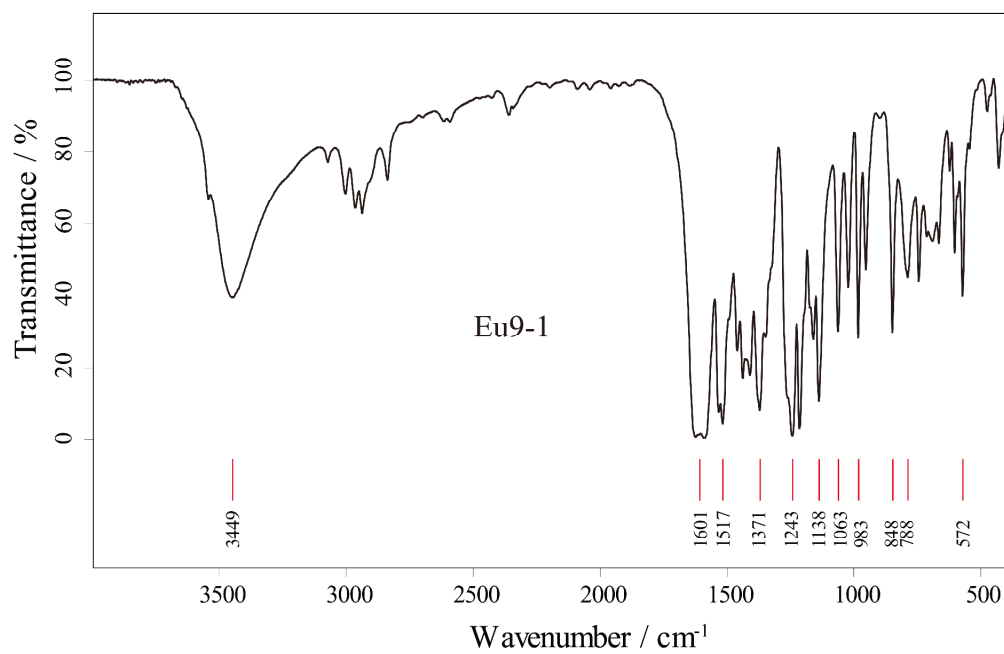
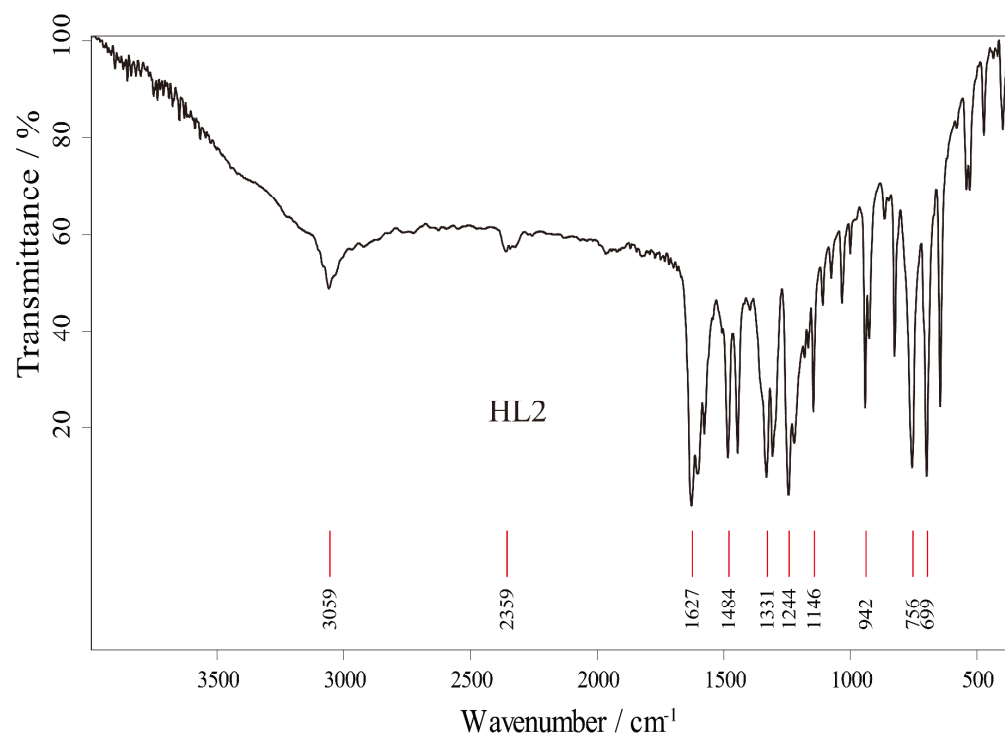
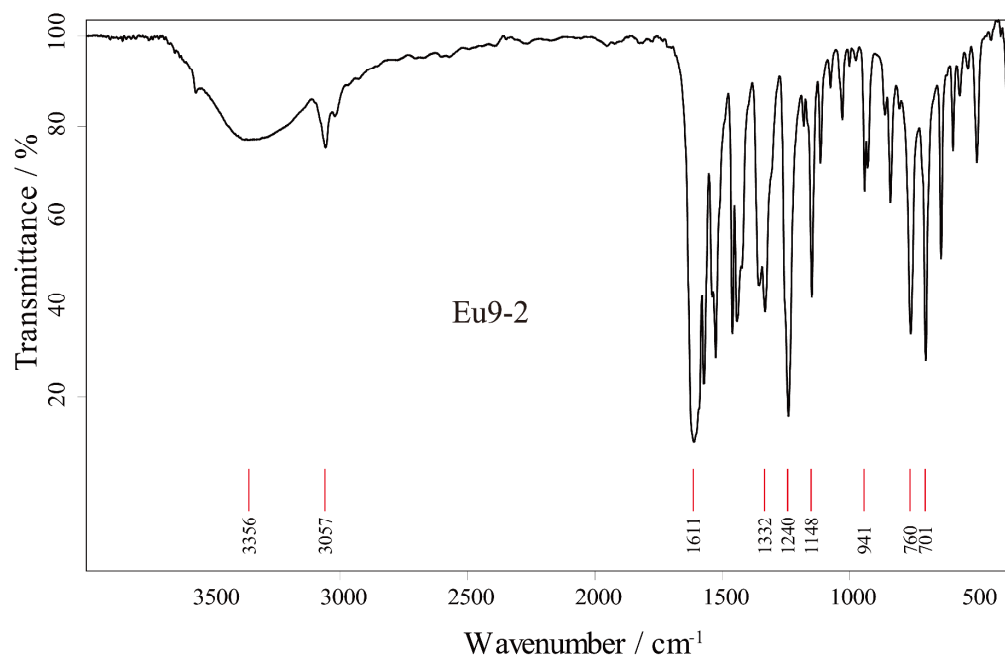


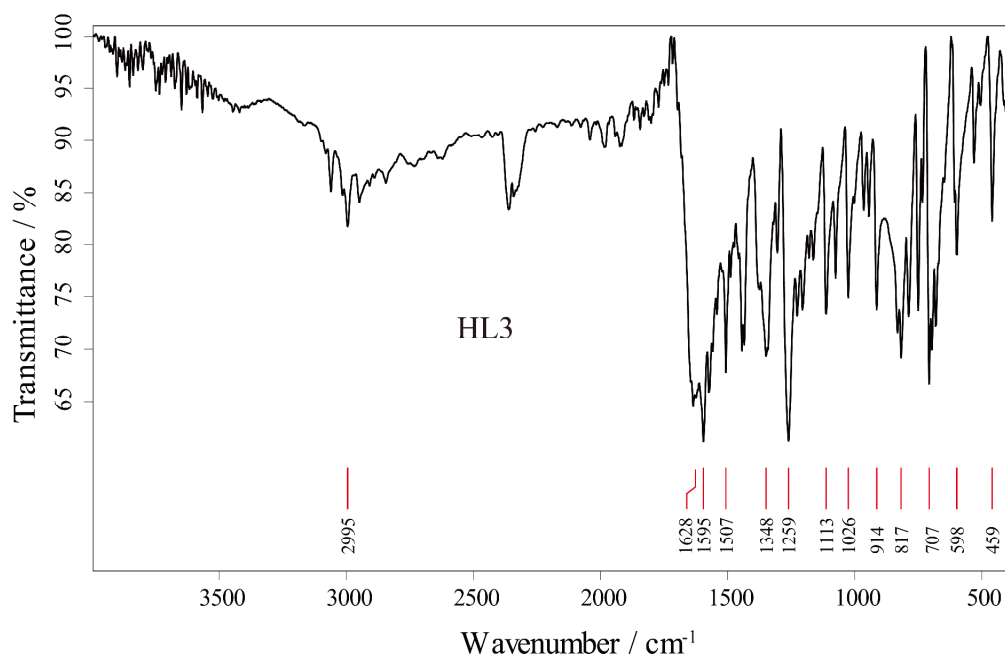
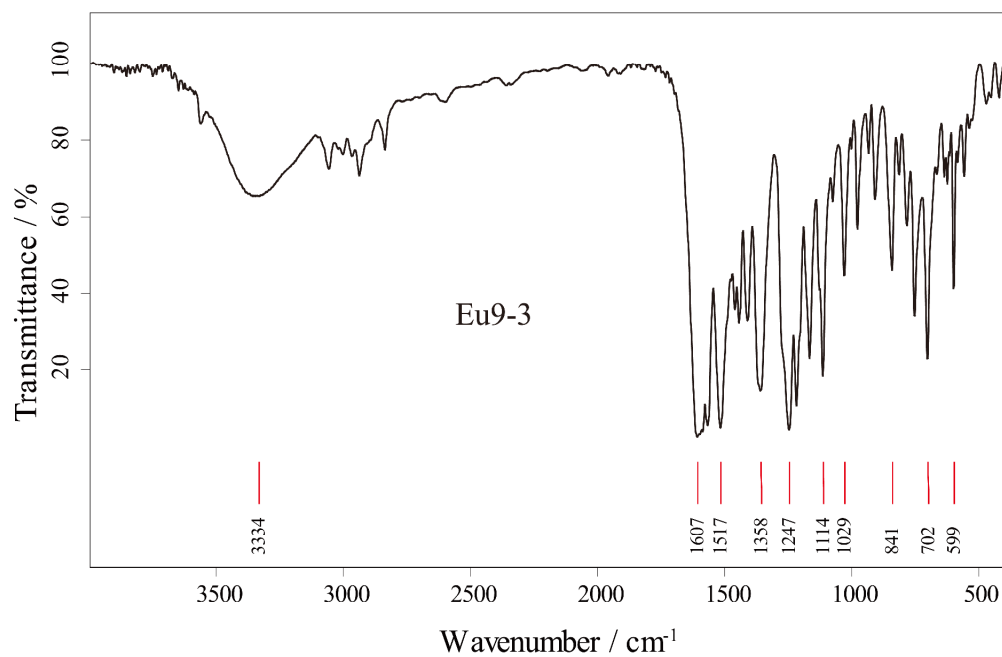
Figure S2. Representation of two vertex-sharing square pyramids formed by the europium ions.

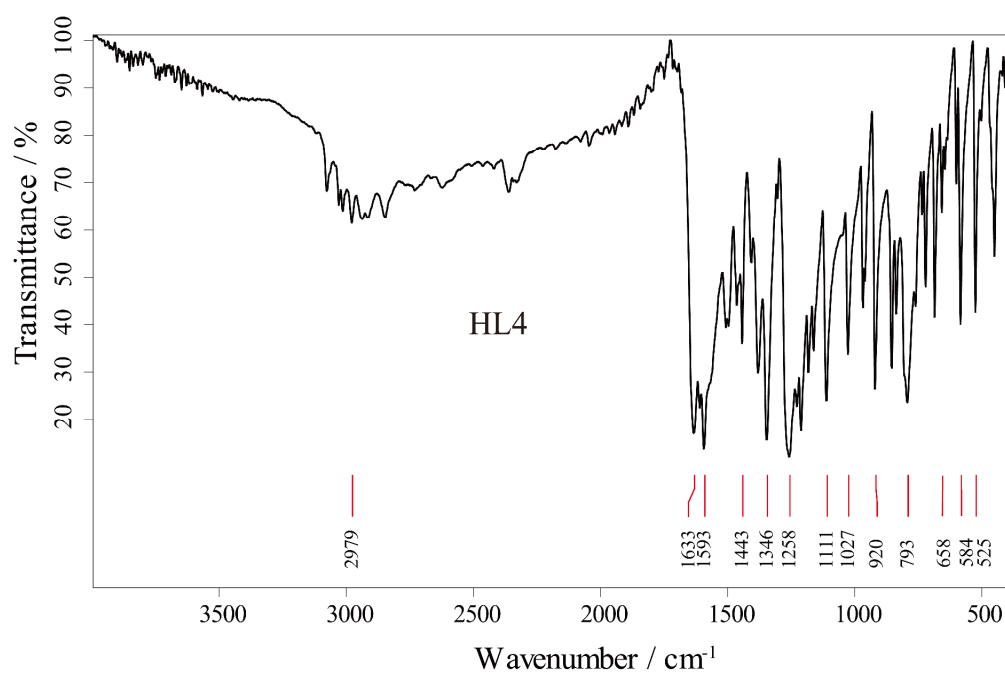
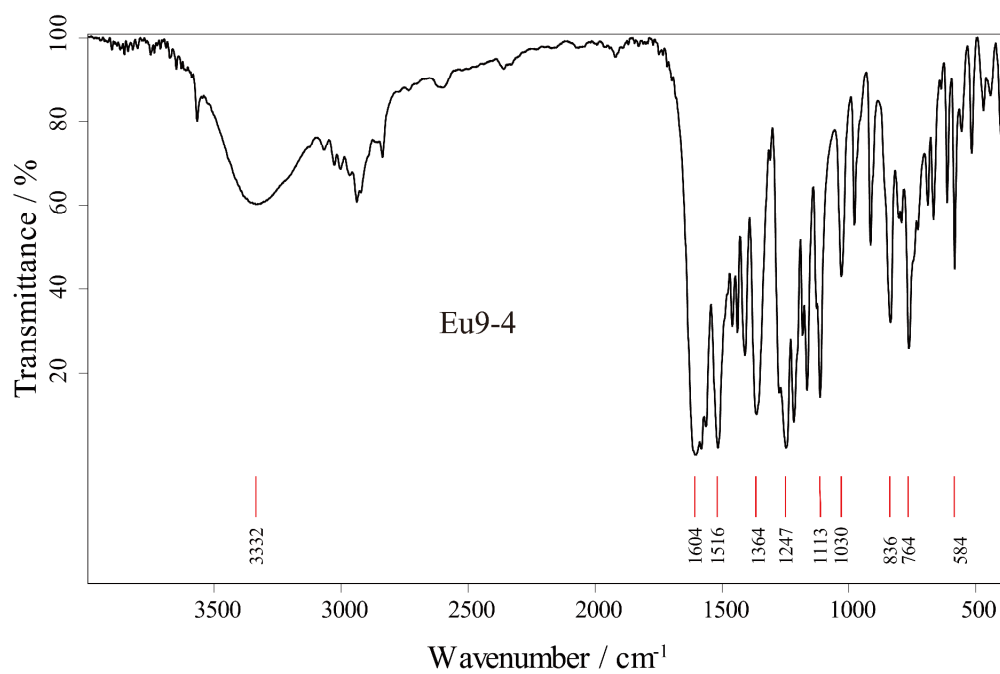
Table S2. Selected bond lengths (Å) and angles (deg) for Eu9-3.

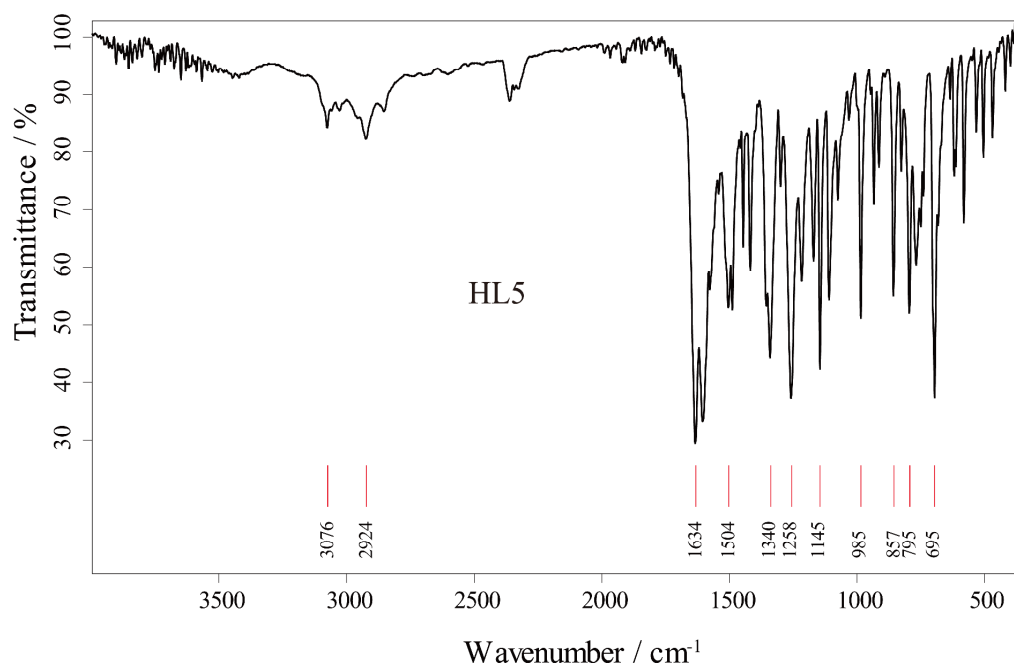
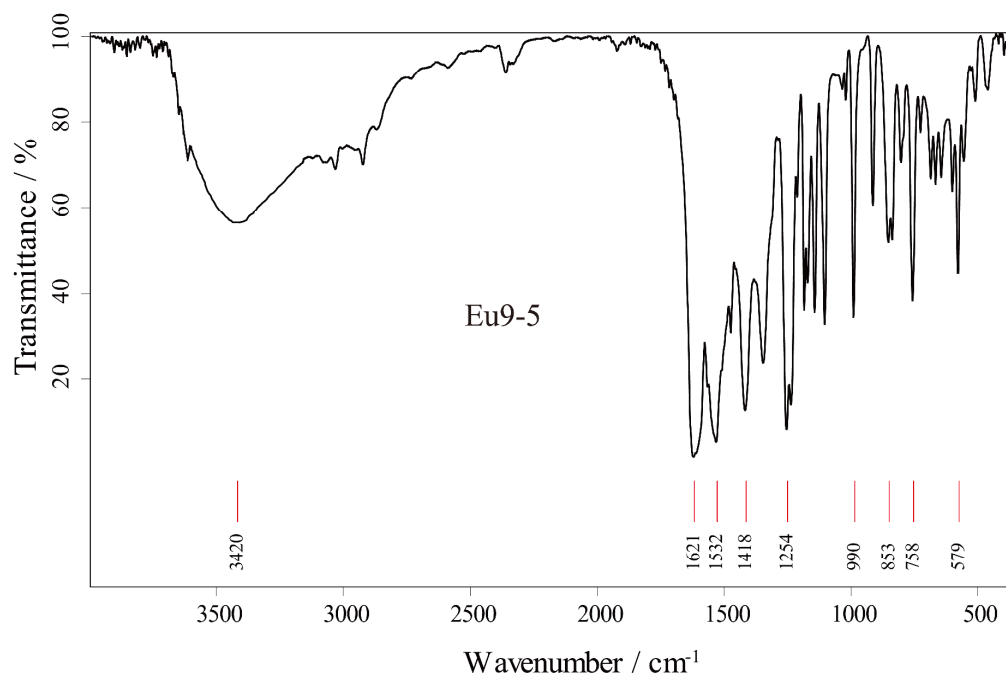
	Distances (Å)		Angles (deg)		Angles (deg)
Eu(1)-O(1)	2.293(3)	O(1)-Eu(1)-O(2)	71.39(11)	O(25)-Eu(5)-O(25)#1	146.45(11)
Eu(1)-O(2)	2.364(3)	O(1)-Eu(1)-O(4)	79.91(11)	O(25)-Eu(5)-O(26)	137.65(7)
Eu(1)-O(4)	2.402(3)	O(1)-Eu(1)-O(5)	133.46(10)	O(25)-Eu(5)-O(26)#1	74.16(8)
Eu(1)-O(5)	2.403(3)	O(1)-Eu(1)-O(19)#1	136.00(10)	O(25)#1-Eu(5)-O(26)	74.15(8)
Eu(1)-O(19)#1	2.453(3)	O(1)-Eu(1)-O(25)#1	80.06(9)	O(25)#1-Eu(5)-O(26)#1	137.65(7)
Eu(1)-O(25)#1	2.336(2)	O(1)-Eu(1)-O(28)	79.04(9)	O(25)-Eu(5)-O(27)	72.30(8)
Eu(1)-O(28)	2.361(3)	O(1)-Eu(1)-O(29)	134.40(9)	O(25)-Eu(5)-O(27)#1	118.18(9)
Eu(1)-O(29)	2.606(2)	O(2)-Eu(1)-O(4)	75.67(12)	O(25)#1-Eu(5)-O(27)	118.18(9)
Eu(2)-O(5)	2.439(3)	O(2)-Eu(1)-O(5)	128.18(11)	O(25)#1-Eu(5)-O(27)#1	72.30(8)
Eu(2)-O(7)	2.361(3)	O(2)-Eu(1)-O(19)#1	72.44(10)	O(25)-Eu(5)-O(28)	78.74(8)
Eu(2)-O(8)	2.288(3)	O(2)-Eu(1)-O(25)#1	91.38(10)	O(25)-Eu(5)-O(28)#1	74.44(8)
Eu(2)-O(10)	2.403(3)	O(2)-Eu(1)-O(28)	150.06(10)	O(25)#1-Eu(5)-O(28)	74.44(8)
Eu(2)-O(11)	2.410(3)	O(2)-Eu(1)-O(29)	134.61(9)	O(25)#1-Eu(5)-O(28)#1	78.75(8)
Eu(2)-O(27)	2.356(2)	O(4)-Eu(1)-O(5)	68.63(10)	O(26)-Eu(5)-O(26)#1	72.33(12)
Eu(2)-O(28)	2.358(2)	O(4)-Eu(1)-O(19)#1	114.09(11)	O(26)-Eu(5)-O(27)	75.63(8)
Eu(2)-O(29)	2.636(2)	O(4)-Eu(1)-O(25)#1	158.80(10)	O(26)-Eu(5)-O(27)#1	77.17(8)
Eu(3)-O(11)	2.437(3)	O(4)-Eu(1)-O(28)	104.05(11)	O(26)#1-Eu(5)-O(27)	77.17(8)
Eu(3)-O(13)	2.382(3)	O(4)-Eu(1)-O(29)	135.34(9)	O(26)#1-Eu(5)-O(27)#1	75.63(8)
Eu(3)-O(14)	2.288(3)	O(5)-Eu(1)-O(19)#1	89.07(10)	O(26)-Eu(5)-O(28)	118.15(9)
Eu(3)-O(22)#1	2.446(3)	O(5)-Eu(1)-O(25)#1	131.61(9)	O(26)-Eu(5)-O(28)#1	145.53(8)
Eu(3)-O(23)#1	2.383(3)	O(5)-Eu(1)-O(28)	76.55(9)	O(26)#1-Eu(5)-O(28)	145.53(8)
Eu(3)-O(26)	2.340(2)	O(5)-Eu(1)-O(29)	66.72(8)	O(26)#1-Eu(5)-O(28)#1	118.15(9)
Eu(3)-O(27)	2.350(2)	O(19)#1-Eu(1)-O(25)#1	76.60(9)	O(27)-Eu(5)-O(27)#1	146.14(11)
Eu(3)-O(29)	2.571(2)	O(19)#1-Eu(1)-O(29)	64.71(8)	O(27)-Eu(5)-O(28)	74.55(8)
Eu(4)-O(16)	2.298(3)	O(25)#1-Eu(1)-O(28)	78.79(8)	O(27)-Eu(5)-O(28)#1	137.22(8)
Eu(4)-O(17)	2.382(3)	O(25)#1-Eu(1)-O(29)	65.35(8)	O(27)#1-Eu(5)-O(28)	137.22(8)
Eu(4)-O(19)	2.422(3)	O(28)-Eu(1)-O(19)#1	130.68(9)	O(27)#1-Eu(5)-O(28)#1	74.55(8)
Eu(4)-O(20)	2.418(3)	O(28)-Eu(1)-O(29)	66.26(8)	O(28)-Eu(5)-O(28)#1	73.21(12)
Eu(4)-O(22)	2.509(3)				
Eu(4)-O(25)	2.371(2)				
Eu(4)-O(26)#1	2.338(3)				
Eu(4)-O(29)#1	2.575(2)				
Eu(5)-O(25)	2.472(2)				
Eu(5)-O(25)#1	2.472(2)				
Eu(5)-O(26)	2.466(2)				
Eu(5)-O(26)#1	2.466(2)				
Eu(5)-O(27)	2.455(2)				
Eu(5)-O(27)#1	2.455(2)				
Eu(5)-O(28)	2.457(2)				
Eu(5)-O(28)#1	2.457(2)				













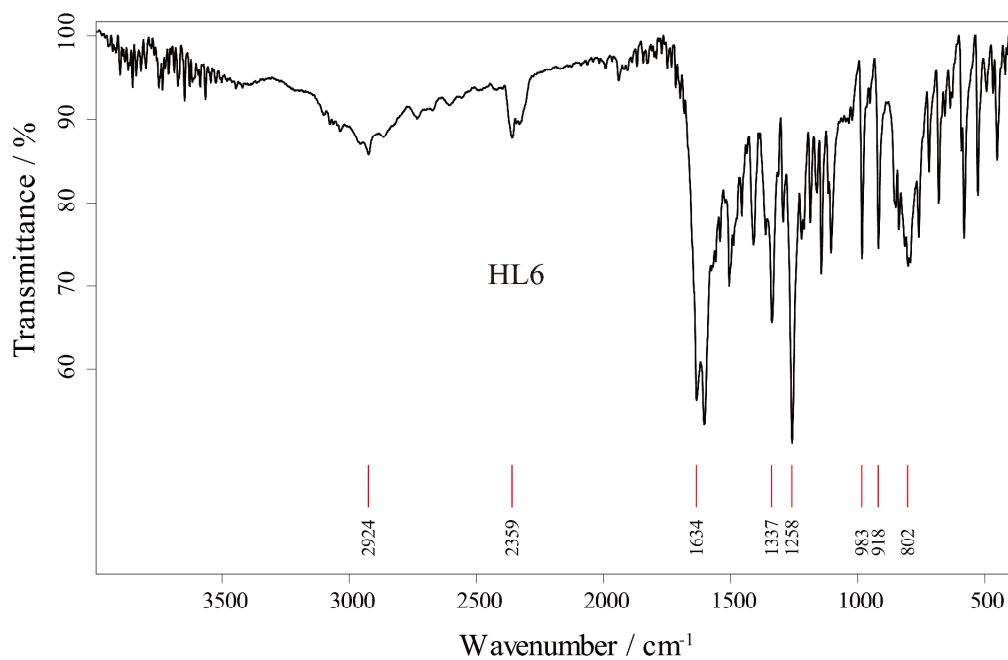
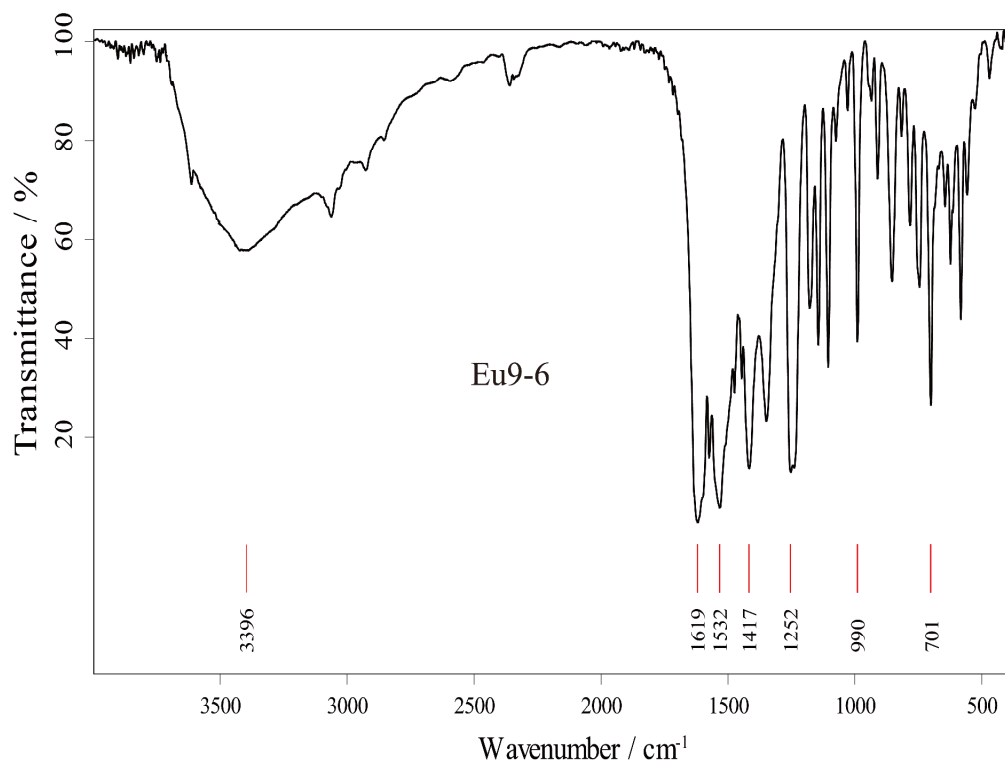


Figure S3. IR spectra of the free ligands and the related complexes.

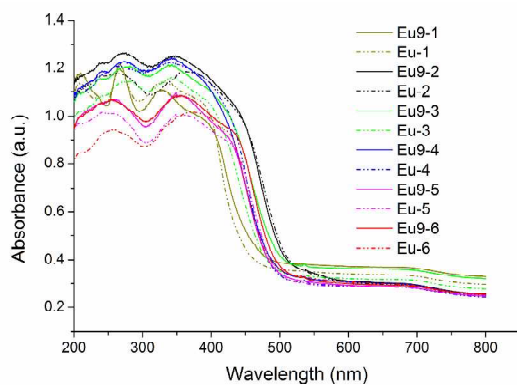


Figure S4. The absorption spectra of the mononuclear europium complexes and nonanuclear clusters in solid state at 298 K.

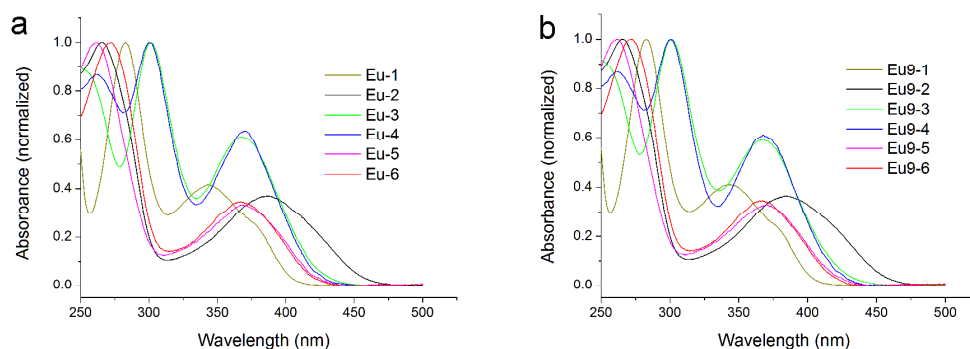


Figure S5. The absorption spectra for both the mononuclear europium complexes (a) and nonanuclear clusters (b) in acetonitrile solution ( $c = 2.0 \times 10^{-5} \text{ mol} \cdot \text{cm}^{-3}$ ). The concentrations of the complexes were based on Eu(III) ion. All spectra are normalized to a constant intensity at the maximum.

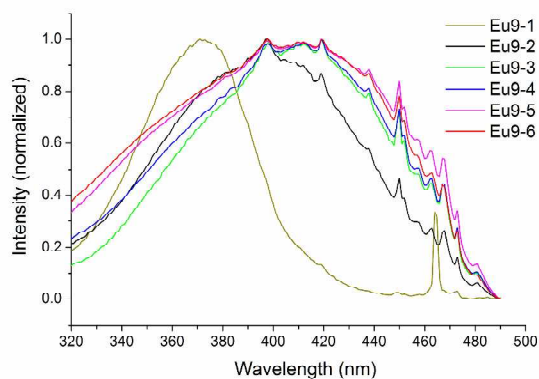


Figure S6. Normalized excitation spectra of complexes Eu9-1 to Eu9-6 at 298 K in the solid state.

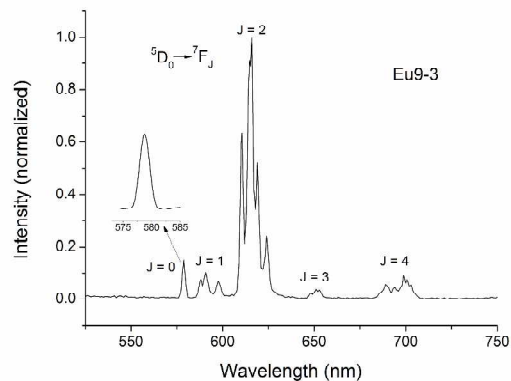


Figure S7. Luminescence spectrum of the cluster Eu9-3 at 77 K in solid-state. high-resolution scan of the  $^5D_0 \rightarrow ^7F_0$  transition is given in the inset.

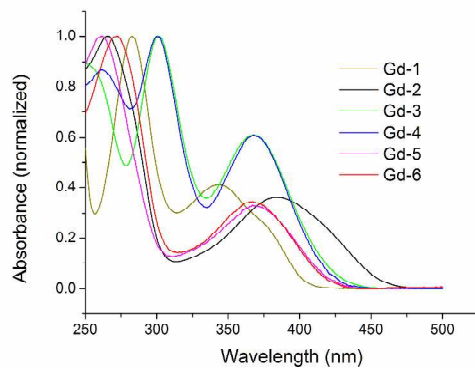


Figure S8. UV-Vis absorption spectra of the mononuclear gadolinium complexes in acetonitrile solution ( $c = 2.0 \times 10^{-5} \text{ mol} \cdot \text{cm}^{-3}$ ). All spectra are normalized to a constant intensity at the maximum.

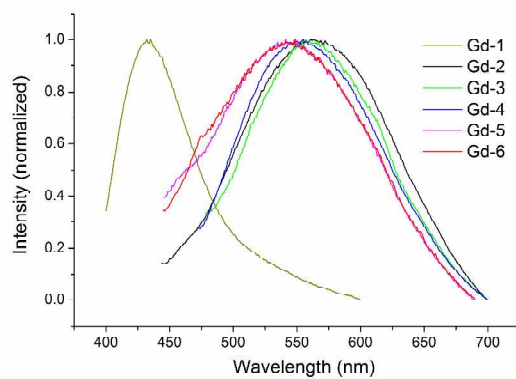


Figure S9. Phosphorescence spectra of the gadolinium complexes  $\text{Gd}(\text{L})_3(\text{H}_2\text{O})_2$  at 77 K.

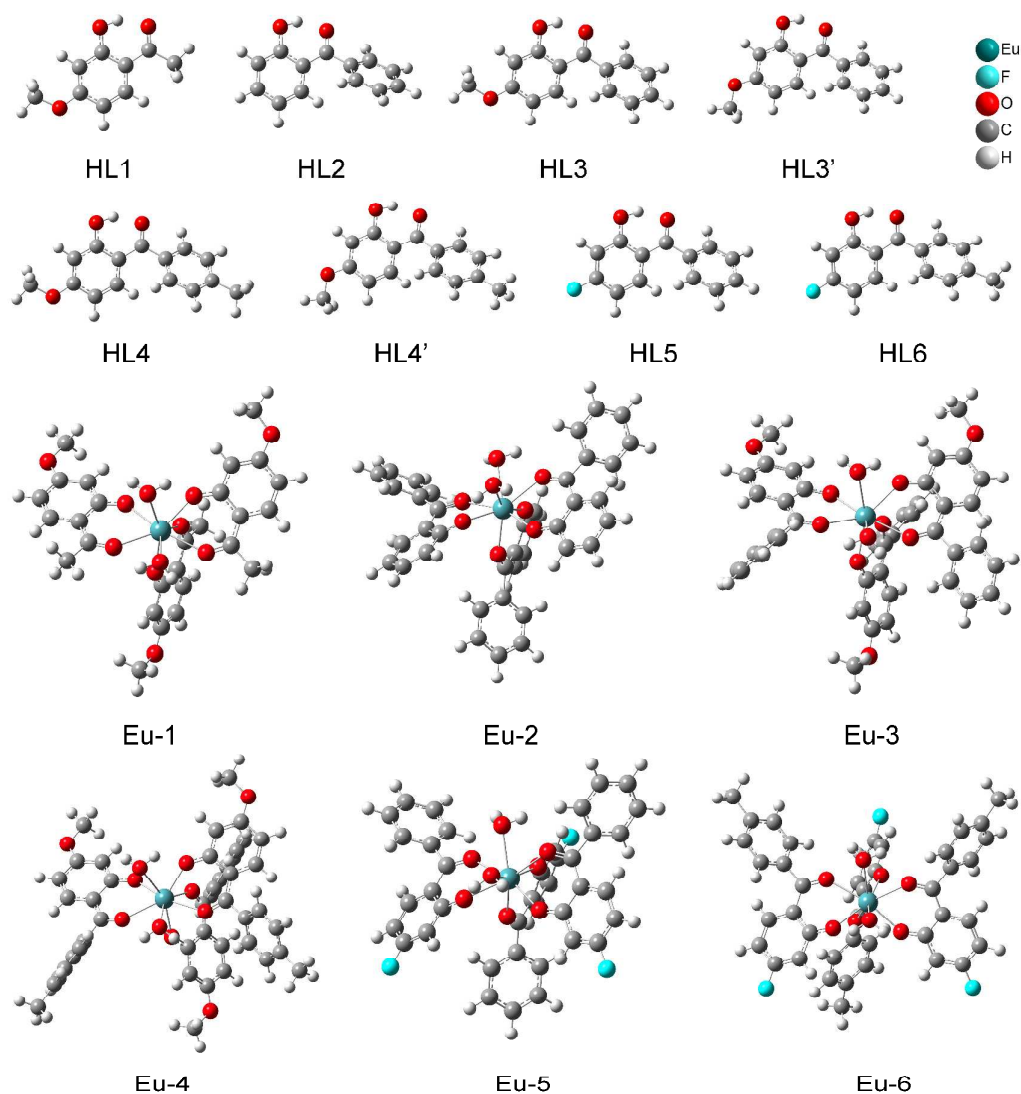


Figure S10. The optimized geometrical structures of the ligands and europium complexes.

Table S3. Cartesian coordinates of HL1 and HL2 from B3LYP calculation.

HL1				HL2			
O	0.70084400	2.18722600	-0.00076400	O	-2.52609900	1.97366000	0.45412700
O	3.00968000	1.07921200	0.00103400	O	0.00761000	2.13296700	0.05342800
O	-3.10627800	-0.67580000	0.00039600	C	-2.39131200	0.67120300	0.16973600
C	0.19993300	0.94653900	-0.00045600	C	-3.55454500	-0.11055700	0.13009800
C	-1.19500600	0.81585200	-0.00013900	H	-4.50038700	0.37078500	0.34665000
H	-1.78191200	1.72326600	-0.00026200	C	-3.48257000	-1.45187300	-0.20354000
C	-1.77124700	-0.44914700	-0.00008200	C	-2.25255900	-2.05071800	-0.50898600
C	-0.96232400	-1.60543600	-0.00035900	H	-2.20753600	-3.09343600	-0.79830100
H	-1.44003800	-2.57643000	-0.00035400	C	-1.09615700	-1.29458000	-0.44354100
C	0.40578600	-1.46928600	-0.00046400	H	-0.14728300	-1.74937300	-0.69539100
H	1.01649700	-2.36372400	-0.00051400	C	-1.12613200	0.06911000	-0.08282800

C	1.03525300	-0.20376400	-0.00050800	C	0.08997700	0.89763600	-0.00367500
C	2.48911900	-0.04585400	0.00015900	C	1.45598900	0.28492500	0.01442200
C	3.38774200	-1.26452200	0.00023200	C	2.47470400	0.92350000	-0.70519100
H	4.42384900	-0.93033400	0.00102300	H	2.23443100	1.80856600	-1.28161400
H	3.20831100	-1.88408900	-0.88275200	C	3.77265000	0.42594100	-0.67755300
H	3.20722800	-1.88479800	0.88236400	H	4.55069000	0.91601500	-1.25172800
C	-3.99599800	0.43825700	0.00053000	C	4.07571900	-0.69386500	0.09794200
H	-4.99826100	0.01428500	0.00029000	H	5.09030500	-1.07487400	0.12846800
H	-3.85865000	1.05341600	-0.89385400	C	3.07465000	-1.31581200	0.84170500
H	-3.85878100	1.05293700	0.89526400	H	3.31076400	-2.17242300	1.46272400
H	1.68823700	2.09453800	-0.00000800	C	1.76748400	-0.83643500	0.79373200
				H	0.99772700	-1.31516600	1.38664600
				H	-1.63486300	2.38550800	0.35132600
				H	-4.39331200	-2.03946200	-0.24314100

Table S4. Cartesian coordinates of HL3 and HL3' from B3LYP calculation.

HL3				HL3'			
O	-1.43001800	2.49699800	0.41624700	O	-1.23508600	2.79528700	0.38505200
O	1.09002000	2.24986200	0.07561700	O	1.25118100	2.29189500	-0.01419500
O	-4.12172300	-1.37828000	-0.21922100	O	-4.34859500	-0.65286600	-0.01427300
C	-1.50588000	1.18386500	0.17046900	C	-1.44131100	1.48673200	0.18726600
C	-2.78359700	0.61142500	0.13818600	C	-2.75530500	1.02767000	0.19968200
H	-3.62654500	1.26137000	0.32491600	H	-3.56305300	1.72577000	0.37623400
C	-2.92939400	-0.74010000	-0.15330800	C	-3.03585200	-0.31535000	-0.03961900
C	-1.79905100	-1.53989900	-0.42174300	C	-1.99476300	-1.22581300	-0.30277500
H	-1.94512800	-2.58143300	-0.67668500	H	-2.19699500	-2.26430700	-0.52199900
C	-0.54543700	-0.97788400	-0.36477700	C	-0.68902800	-0.76934500	-0.28809100
H	0.31432700	-1.59387000	-0.59230400	H	0.10620000	-1.46861000	-0.50975300
C	-0.34656400	0.38626000	-0.04669100	C	-0.36143100	0.57357100	-0.02481000
C	0.97403100	1.01310700	0.01810500	C	1.01642300	1.07248600	-0.01162900
C	2.23067500	0.19695800	0.01879300	C	2.18818200	0.13788600	0.00449400
C	3.31487500	0.65197900	-0.74276500	C	2.25263200	-0.97334900	0.85421100
H	3.19847200	1.55060000	-1.33637200	H	1.42140800	-1.20227900	1.51018000
C	4.52095000	-0.04021400	-0.73324400	C	3.40003600	-1.76311200	0.89110900
H	5.34878500	0.31032800	-1.33913600	H	3.44878300	-2.60989400	1.56635400
C	4.66937700	-1.17567400	0.06405300	C	4.48325800	-1.46263800	0.06750800
H	5.61329500	-1.70887800	0.07988900	H	5.37141900	-2.08407900	0.09050700
C	3.60549800	-1.61700400	0.84853000	C	4.42677000	-0.35456000	-0.77872400
H	3.72352400	-2.48579400	1.48616000	H	5.27037700	-0.11359800	-1.41554300
C	2.38749100	-0.94083600	0.81997500	C	3.29355900	0.45112000	-0.79708600
H	1.57059400	-1.27954200	1.44572900	H	3.25084500	1.32999000	-1.42894900
C	-5.31587300	-0.63871400	0.02567200	C	-4.72490800	-2.00430100	-0.26308700
H	-5.43782900	0.16705600	-0.70457000	H	-4.29249000	-2.68110300	0.48042900

H	-5.32273300	-0.22301600	1.03786100	H	-4.42864100	-2.32131500	-1.26790000
H	-6.13075500	-1.35218100	-0.08024000	H	-5.81012800	-2.02574200	-0.18318100
H	-0.47484200	2.74711800	0.32608900	H	-0.26731100	2.95466000	0.26024700

Table S5. Cartesian coordinates of HL4 and HL4' from B3LYP calculation.

HL4				HL4'			
O	-2.01496800	2.46967700	0.43286500	O	1.89843200	2.76019400	-0.41357700
O	0.51088300	2.42429400	0.06854600	O	-0.61914000	2.52124200	0.02649100
C	-0.86842700	-0.91879300	-0.38394100	C	0.99670500	-0.72051200	0.31071800
H	0.03482600	-1.46305500	-0.62556600	H	0.13657900	-1.33160000	0.55013700
C	-1.98970600	1.15618800	0.17755100	C	1.97143600	1.43943600	-0.20156100
C	-0.77339000	0.45331900	-0.05368900	C	0.80567600	0.64496000	0.03134200
C	0.49586800	1.18157000	0.00985900	C	-0.51492800	1.28318700	0.02369800
C	-3.21928100	0.48594300	0.14971400	C	3.23144600	0.84778900	-0.22060500
H	-4.10887200	1.06668900	0.34769500	H	4.10439300	1.45741300	-0.41395200
C	-3.26177600	-0.87032600	-0.15213600	C	3.37525100	-0.51375800	0.03433400
O	-4.40144900	-1.59961600	-0.21447600	O	4.64620600	-0.98600500	0.00101400
C	1.81096700	0.46905400	0.00682800	C	-1.77519800	0.47702500	0.01236600
C	2.05786900	-0.67702700	0.77384700	C	-1.95402000	-0.64257800	-0.80667000
H	1.26893500	-1.10276100	1.38222000	H	-1.14852700	-0.98079800	-1.44739500
C	-2.07495700	-1.57671800	-0.43690100	C	2.24919300	-1.30841900	0.32035900
H	-2.14143600	-2.62398000	-0.70168700	H	2.34634000	-2.35896800	0.55349400
C	3.32405100	-1.25232000	0.79427800	C	-3.17968800	-1.30488700	-0.83927500
H	3.49894600	-2.12997600	1.40867200	H	-3.30428900	-2.16049700	-1.49497000
C	2.86634800	1.02643000	-0.72408900	C	-2.85588800	0.92226600	0.78644400
H	2.68970100	1.92949200	-1.29594100	H	-2.73201200	1.80680700	1.39956000
C	4.12204200	0.42980200	-0.71991900	C	-4.06476200	0.24107500	0.76900900
H	4.92122800	0.86592100	-1.31037600	H	-4.88305500	0.59086500	1.39057300
C	4.37537200	-0.71753100	0.04026700	C	-4.25077700	-0.88399900	-0.04677300
C	-5.64763000	-0.95767300	0.04517200	C	4.88066700	-2.36736700	0.25835200
H	-5.67845400	-0.54963200	1.06011300	H	4.56307800	-2.64368900	1.26864400
H	-6.40496300	-1.73233800	-0.05867300	H	5.95670800	-2.50386000	0.16833500
H	-5.83922400	-0.15957600	-0.67861700	H	4.37121600	-3.00033700	-0.47492400
C	5.74501900	-1.34924000	0.07093100	C	-5.57839100	-1.59960500	-0.07819300
H	6.23803700	-1.16791700	1.03180200	H	-6.35197700	-0.96999700	-0.52974400
H	6.38793500	-0.94470800	-0.71302400	H	-5.91586300	-1.85232100	0.93104600
H	5.68602200	-2.43278100	-0.06347100	H	-5.52080800	-2.52334700	-0.65694600
H	-1.08263900	2.79371900	0.33473300	H	0.95390700	3.01919400	-0.27653500

Table S6. Cartesian coordinates of HL5 and HL6 from B3LYP calculation.

HL5				HL6			
F	-4.46418400	-1.51855400	-0.16462400	F	-4.72320900	-1.81047000	-0.14943500
O	-1.93265800	2.37299000	0.44402200	O	-2.52738100	2.27924200	0.46578600

O	0.59202300	2.23395700	0.03840800	O	-0.00748800	2.36189400	0.02674400
C	-1.95388600	1.06169900	0.18859900	C	-2.43838700	0.97251900	0.20054700
C	-3.20181800	0.42639700	0.17126000	C	-3.62742000	0.23257200	0.19076400
H	-4.10074300	0.99330900	0.37314100	H	-4.56938400	0.71884600	0.40635200
C	-3.25694300	-0.91583800	-0.13495100	C	-3.57109000	-1.10700700	-0.12668900
C	-2.12959100	-1.68008100	-0.43354200	C	-2.38622000	-1.76889100	-0.44476100
H	-2.23544400	-2.72369100	-0.69757100	H	-2.40498000	-2.81519100	-0.71853000
C	-0.89815900	-1.05326700	-0.38702200	C	-1.21237900	-1.03878700	-0.40508600
H	-0.01168100	-1.62214700	-0.63273300	H	-0.28364200	-1.52700000	-0.66733700
C	-0.76606700	0.31069200	-0.05581500	C	-1.19319500	0.32807500	-0.06161400
C	0.53504100	0.99574400	-0.00168800	C	0.04602700	1.12273000	-0.01213800
C	1.82273500	0.23334700	0.01031500	C	1.39234200	0.47649700	-0.00476700
C	2.89597500	0.74033100	-0.73448100	C	2.42879300	1.09530100	-0.71877600
H	2.74847200	1.63646600	-1.32478700	H	2.21216600	1.99258500	-1.28573900
C	4.13000400	0.10033800	-0.71311000	C	3.71065300	0.56557600	-0.70161000
H	4.94979600	0.48959500	-1.30594900	H	4.49454800	1.04835700	-1.27658600
C	4.31644200	-1.03272200	0.07977700	C	4.01336000	-0.57558300	0.05546200
C	3.26307700	-1.52470800	0.84805200	C	2.98370900	-1.16828000	0.79111600
H	3.41064400	-2.39100700	1.48269200	H	3.19668000	-2.03798700	1.40374800
C	2.01757500	-0.90184400	0.80744300	C	1.68738900	-0.65895300	0.75744600
H	1.20928400	-1.27864000	1.42240300	H	0.91585700	-1.12856700	1.35553700
H	-0.99605500	2.67179500	0.33105900	C	5.41528800	-1.13085100	0.07959900
H	5.28216100	-1.52479800	0.10490600	H	5.76063000	-1.37190700	-0.93016600
				H	5.47562800	-2.03880400	0.68228700
				H	6.11846900	-0.40305300	0.49637400
				H	-1.62135700	2.65836300	0.34177000

Table S7. Cartesian coordinates of complexes Eu-1 and Eu-2.

Eu-1				Eu-2			
Eu	0.14624000	-0.18464100	-0.85061700	Eu	0.38324900	-0.35622400	-0.70737200
O	-1.15057500	-1.79125600	0.11017500	O	1.79283400	1.32168700	-1.26662500
O	-1.94185100	-0.58982200	-2.20345700	O	2.75947300	-1.07876700	-0.41475100
O	-1.04601700	1.70129900	-0.42177400	O	0.57222400	-0.33964200	1.55553900
O	0.56867300	0.49210600	1.39383500	O	-0.95287400	1.42824500	0.17776000
O	2.27026300	-1.10887700	-0.57922000	O	-1.14404500	-0.18181000	-2.46127100
O	1.87711400	1.50660600	-1.26637100	O	-1.70342300	-1.56271700	-0.17338700
O	-4.36915800	-4.56131600	2.25112800	C	3.03651500	1.63784600	-1.39945200
O	-3.06956700	5.78426200	0.94670900	C	3.37477300	2.89406200	-1.98254900
O	6.58431000	-2.19967600	1.10932600	H	2.55085000	3.53385600	-2.27617100
C	-2.33828600	-2.29600200	0.11667200	C	4.68346100	3.27689100	-2.16942200
C	-2.70182700	-3.15903100	1.18876700	C	5.74728900	2.43447200	-1.78844400
H	-1.94668200	-3.32509300	1.94415700	H	6.77411800	2.73345700	-1.95982200
C	-3.95502300	-3.73684800	1.25514600	C	5.46166400	1.22188300	-1.20282100

C	-4.91831200	-3.49007700	0.24626600	H	6.27637900	0.56413200	-0.92938000
H	-5.89217400	-3.95524300	0.32505700	C	4.12767200	0.78752100	-0.97916100
C	-4.58815700	-2.66781200	-0.79796000	C	3.87403100	-0.51351800	-0.38841300
H	-5.33648300	-2.48848300	-1.55935900	C	4.97425200	-1.27727600	0.29267900
C	-3.31614600	-2.04249400	-0.91570800	C	5.76711700	-0.69623100	1.28896900
C	-3.02643600	-1.19440400	-2.04625200	H	5.62646100	0.34644300	1.54770500
C	-3.46879900	-4.85869300	3.31361800	C	6.71442300	-1.46040100	1.96735300
H	-4.01206200	-5.52194500	3.98446700	H	7.31058300	-1.00587700	2.75053200
H	-3.17802600	-3.95095500	3.85135600	C	6.89463000	-2.80351900	1.64182300
H	-2.57288100	-5.36651300	2.94284500	H	7.63987600	-3.39390500	2.16298000
C	-1.21560500	2.59273400	0.49490100	C	6.11078700	-3.38770700	0.64650800
C	-2.05496900	3.70798500	0.21200100	H	6.24917800	-4.43162200	0.38825000
H	-2.50326200	3.73234400	-0.77137600	C	5.14478000	-2.63350500	-0.01249900
C	-2.28207200	4.69537100	1.15115000	H	4.52365600	-3.08648800	-0.77674400
C	-1.68360600	4.62613200	2.43278700	C	-0.08041300	0.08588200	2.58666800
H	-1.88097100	5.41400700	3.14788600	C	0.12026300	-0.54487100	3.84855000
C	-0.87477000	3.56057200	2.72831400	H	0.83925300	-1.35535800	3.88391600
H	-0.42450800	3.51927600	3.71200600	C	-0.57585300	-0.15715400	4.97210800
C	-0.60333600	2.51914900	1.80057600	C	-1.51317100	0.89231700	4.91658300
C	0.25831000	1.42271100	2.16943400	H	-2.07641700	1.17472000	5.79767500
C	-3.71867500	5.93318900	-0.31074700	C	-1.70535100	1.55274100	3.72210700
H	-4.28335200	6.86168400	-0.24446000	H	-2.43660700	2.34925100	3.67107200
H	-4.40352900	5.10145100	-0.50430200	C	-1.00393500	1.19406500	2.54314900
H	-2.99174500	6.00459100	-1.12619600	C	-1.23940000	1.90488200	1.29608200
C	3.46507300	-0.71791900	-0.26442100	C	-1.85227100	3.27271300	1.28780900
C	4.37621100	-1.67905200	0.25283400	C	-1.47584400	4.26574000	2.20136000
H	3.99867500	-2.68548900	0.36841800	H	-0.74443900	4.04248000	2.96836400
C	5.66890000	-1.33444600	0.60117300	C	-2.01279500	5.54756300	2.10666100
C	6.12706600	-0.00516800	0.44248000	H	-1.70209700	6.31403200	2.80770900
H	7.14347200	0.23756900	0.72368500	C	-2.94320300	5.84446800	1.11222800
C	5.26823200	0.93444000	-0.06467800	H	-3.36765400	6.84015000	1.04595500
H	5.63388700	1.94636900	-0.18298300	C	-3.31972500	4.86126700	0.19642200
C	3.92772700	0.63724700	-0.43037900	H	-4.03881600	5.09031900	-0.58193900
C	3.08472500	1.66882800	-0.99068300	C	-2.76526400	3.58823300	0.27238000
C	6.21033900	-3.55986600	1.30053700	H	-3.03224700	2.82669700	-0.45006300
H	7.09026500	-4.05403400	1.70878900	C	-2.43272200	-0.05236800	-2.54857700
H	5.93315500	-4.03151500	0.35243800	C	-2.98507500	0.75379000	-3.58186700
H	5.38016900	-3.64660400	2.00861300	H	-2.28795200	1.23182200	-4.26035300
O	0.12378200	0.67792900	-3.23153900	C	-4.34401000	0.95001400	-3.70071100
H	0.32589600	1.62025400	-3.21142500	C	-5.24316800	0.34468800	-2.80311200
O	0.65150600	-2.39347400	-2.18268000	H	-6.30830000	0.52322300	-2.88592300
H	1.51784500	-2.42315600	-1.73649300	C	-4.74636300	-0.47641200	-1.81362100
H	0.10950100	-3.07305600	-1.76634700	H	-5.43238700	-0.93419800	-1.11234400



H	-0.82153000	0.57008500	-3.42001800	C	-3.35656100	-0.71017800	-1.65902000
C	3.66249800	3.04390300	-1.28628400	C	-2.87331600	-1.59341400	-0.60776700
H	3.99855200	3.53339400	-0.36802700	C	-3.77849200	-2.61554100	0.01346800
H	4.51897700	2.98399700	-1.96232400	C	-3.69017500	-2.83257800	1.39547400
H	2.88362700	3.65373900	-1.74100400	H	-3.01378500	-2.22247600	1.98207100
C	0.84999500	1.34969200	3.56720900	C	-4.46942400	-3.81012200	2.00496200
H	1.48600400	2.21483400	3.77335700	H	-4.40949600	-3.95650200	3.07752200
H	0.06697900	1.32517500	4.32953200	C	-5.32184100	-4.60450400	1.23698400
H	1.44910600	0.44356200	3.63711300	H	-5.92187600	-5.37328100	1.71098000
C	-4.07010800	-1.00126800	-3.13493400	C	-5.39701200	-4.41171800	-0.14138400
H	-4.36766900	-1.95420100	-3.57919900	H	-6.04572100	-5.03763700	-0.74370800
H	-4.97003100	-0.52535100	-2.73611500	C	-4.63792100	-3.41511600	-0.75070400
H	-3.64988100	-0.36376600	-3.91121900	H	-4.69399200	-3.27267300	-1.82302500
				O	0.74797000	-2.83481300	-0.31510800
				H	0.12101100	-3.12949700	0.35592700
				O	1.20019400	-1.10205100	-3.08526200
				H	0.36095100	-0.77861400	-3.46108700
				H	1.90136400	-0.55712800	-3.45725700
				H	1.63357700	-2.83834700	0.07553800
				H	4.89819700	4.23930200	-2.62344500
				H	-4.72330900	1.58930200	-4.49180600
				H	-0.40396500	-0.67393500	5.91133300

Table S8. Cartesian coordinates of complexes Eu-3 and Eu-4.

Eu-3				Eu-4			
Eu	0.34759600	0.08432200	-0.88598100	Eu	0.41535800	-0.01388800	-0.92479600
O	1.85564400	1.62098300	-0.14816000	O	1.78771100	1.75867100	-0.53161300
O	2.66537600	-0.67703900	-1.36816900	O	2.79673500	-0.70276300	-1.12170000
O	0.54536900	-1.54911800	0.68487800	O	0.62824700	-1.20054500	1.00428700
O	-0.85748100	0.74141200	1.06078400	O	-0.92733300	1.00734900	0.75690800
O	-1.27465600	1.46350100	-1.86115400	O	-1.23343000	0.96969300	-2.26601300
O	-1.74776100	-1.15552400	-1.24895600	O	-1.57989500	-1.45023800	-1.04872000
O	5.29678400	4.68888100	1.01332700	O	4.97289700	5.25272200	-0.03292200
O	-0.35232500	-5.06224600	3.76875200	O	-0.21729100	-3.91795100	4.81991000
O	-5.09018500	4.31188200	-1.85419800	O	-5.20817300	3.45690100	-3.09474900
C	3.11470700	1.88391100	-0.07115200	C	3.02295400	2.12111400	-0.47582200
C	3.51469200	3.14840400	0.44560200	C	3.31868800	3.49816200	-0.27028200
H	2.71842200	3.80769000	0.76163900	H	2.46881500	4.15607600	-0.15431300
C	4.84810600	3.50034500	0.53598000	C	4.62200100	3.95525400	-0.22064100
C	5.86296800	2.60795600	0.11017500	C	5.70951400	3.06073000	-0.37797800
H	6.89673500	2.92250100	0.16879000	H	6.71804200	3.45268000	-0.36079800
C	5.50567600	1.37781800	-0.37308400	C	5.45252000	1.72806100	-0.55793300
H	6.28547800	0.71080700	-0.71623000	H	6.28786100	1.05494500	-0.69887100

C	4.14976700	0.95612000	-0.47625000	C	4.13164100	1.19877400	-0.60369800
C	3.82268000	-0.33550300	-1.02423500	C	3.91183800	-0.20690700	-0.83021700
C	4.88732600	-1.37710900	-1.23382000	C	5.04660500	-1.18999100	-0.73972500
C	5.74530200	-1.77425900	-0.20196800	C	5.87162900	-1.26380600	0.38830700
H	5.68471300	-1.28760400	0.76435000	H	5.73138900	-0.56342000	1.20321100
C	6.65635600	-2.80944300	-0.40396700	C	6.85250900	-2.24974400	0.47902000
H	7.30461900	-3.12067400	0.40751900	H	7.47487500	-2.30860700	1.36491800
C	6.73372400	-3.44318400	-1.64281000	C	7.03258200	-3.15719600	-0.56330900
H	7.44990700	-4.24163800	-1.80156700	C	6.21549100	-3.08747600	-1.69206100
C	5.88333800	-3.05029600	-2.67676600	H	6.35259200	-3.79011000	-2.50647200
H	5.94065700	-3.53905900	-3.64298600	C	5.21823000	-2.12018700	-1.77253600
C	4.95500200	-2.03468200	-2.46850000	H	4.57120600	-2.07181700	-2.64096000
H	4.28204700	-1.73640400	-3.26430300	C	3.94499100	6.22448300	0.13392500
C	4.34716600	5.65010600	1.46390600	H	4.45703000	7.17530800	0.27118300
H	4.93004100	6.50587700	1.80006700	H	3.33343800	6.00663500	1.01486500
H	3.75396800	5.26030800	2.29678200	H	3.30375400	6.27810500	-0.75145000
H	3.67973900	5.95726900	0.65264700	C	0.00214400	-1.37209100	2.11941600
C	-0.05057200	-1.95057600	1.75661900	C	0.25511800	-2.55399100	2.87115500
C	0.14489600	-3.29354900	2.18581600	H	0.98152300	-3.23930900	2.45703800
H	0.80535800	-3.89894100	1.58074700	C	-0.40274300	-2.80546400	4.06111500
C	-0.48566900	-3.78876900	3.31239000	C	-1.35157700	-1.88761500	4.57133900
C	-1.34786800	-2.96853700	4.07847900	H	-1.87329700	-2.12620000	5.48897900
H	-1.85166400	-3.39278000	4.93719000	C	-1.58765400	-0.72600100	3.88269400
C	-1.52565100	-1.66165700	3.70462000	H	-2.32814800	-0.03698300	4.26745200
H	-2.20095700	-1.04465000	4.28287700	C	-0.93119300	-0.41127400	2.66236900
C	-0.89309000	-1.09770700	2.56400000	C	-1.21518700	0.81913000	1.96149000
C	-1.11419600	0.28161300	2.19743900	C	-1.88771400	1.97070500	2.65092200
C	-1.67789100	1.26755800	3.17922000	C	-1.51039300	2.40014100	3.92930900
C	-1.22502900	1.34746500	4.50194100	H	-0.73658600	1.86776400	4.46902000
H	-0.47194700	0.65368600	4.85553600	C	-2.10127000	3.52766300	4.49618500
C	-1.71347600	2.33524000	5.35488300	H	-1.78946400	3.86145300	5.47957000
H	-1.34338400	2.39875300	6.37207700	C	-3.08703600	4.22526500	3.80053100
C	-2.67175700	3.23981200	4.90127100	C	-3.46580900	3.80487000	2.52492200
H	-3.05886900	4.00170300	5.56889500	H	-4.22983000	4.34684900	1.97877400
C	-3.12532400	3.16806200	3.58350500	C	-2.85818000	2.69555400	1.94628900
H	-3.86820300	3.87212000	3.22548400	H	-3.12765500	2.37930400	0.94595200
C	-2.61931200	2.19977700	2.72269800	C	0.72846900	-4.89081400	4.39037900
H	-2.94657500	2.15484700	1.69110400	H	0.71773000	-5.67002000	5.15072700
C	0.50582500	-5.95528900	3.06769900	H	1.73320500	-4.46253200	4.31884400
H	0.46731700	-6.89485200	3.61646500	H	0.44585400	-5.31990500	3.42363100
H	1.53518100	-5.58363600	3.04934700	C	-2.52769400	1.02991900	-2.24169300
H	0.15866800	-6.11685100	2.04204200	C	-3.16402200	2.21118800	-2.70879500
C	-2.55964900	1.59351800	-1.75520800	H	-2.51467700	3.00124300	-3.05956900

C	-3.12699900	2.88920000	-1.88869100	C	-4.54043800	2.34812500	-2.68223700
H	-2.43632600	3.70064500	-2.07146200	C	-5.35954700	1.30427000	-2.19217900
C	-4.48835700	3.09783300	-1.75771700	H	-6.43140400	1.44921900	-2.15652300
C	-5.36123200	2.01687200	-1.49249400	C	-4.76954700	0.14085800	-1.77028200
H	-6.41810100	2.21275000	-1.36672400	H	-5.39978300	-0.64880800	-1.38266000
C	-4.84043100	0.75232000	-1.39606300	C	-3.36216300	-0.05580400	-1.78603900
H	-5.51069500	-0.06891800	-1.17849800	C	-2.78701100	-1.30843800	-1.34924500
C	-3.45205200	0.48138700	-1.53264200	C	-3.63161700	-2.54567300	-1.23358200
C	-2.95184700	-0.87226200	-1.44258200	C	-3.45623100	-3.36845200	-0.11269900
C	-3.87741200	-2.04715600	-1.58554800	H	-2.75863900	-3.06586800	0.65922800
C	-3.72043400	-3.12833400	-0.70775700	C	-4.17751100	-4.55156900	0.01144400
H	-2.97565000	-3.06640200	0.07679600	H	-4.05147700	-5.16966800	0.89331800
C	-4.51891700	-4.26033800	-0.83587700	C	-5.05724000	-4.94413700	-0.99806800
H	-4.40525300	-5.08196400	-0.13756200	C	-5.21745200	-4.14453900	-2.12838000
C	-5.46024400	-4.34024300	-1.86284700	H	-5.88726100	-4.45369400	-2.92295600
H	-6.07596000	-5.22659600	-1.96822600	C	-4.51691400	-2.94529100	-2.24216400
C	-5.60408200	-3.28010000	-2.75617600	H	-4.64043600	-2.32892100	-3.12459800
H	-6.32245800	-3.34451300	-3.56571800	C	-4.46268200	4.55449600	-3.61123600
C	-4.82475600	-2.13377700	-2.61303000	H	-5.19805300	5.30993700	-3.88277700
H	-4.93605900	-1.31383800	-3.31243800	H	-3.89276300	4.26285200	-4.49912000
C	-4.28783600	5.45573800	-2.12817100	H	-3.78132100	4.96137500	-2.85735200
H	-4.97706600	6.29740700	-2.16999400	O	0.84960100	-2.26143800	-2.00638400
H	-3.77255800	5.35669900	-3.08883800	H	0.24977100	-2.89556600	-1.59522100
H	-3.55248000	5.62398800	-1.33502000	O	1.12178600	0.74099400	-3.33925500
O	0.58177400	-1.85187800	-2.50034500	H	0.23721600	1.13407300	-3.45487000
H	-0.04628700	-2.53019100	-2.22394000	H	1.74997900	1.47047900	-3.31733400
O	1.01800500	1.36359200	-3.07972700	H	1.74981900	-2.44324000	-1.69975600
H	0.15996800	1.82538200	-3.05031300	C	8.12643400	-4.23695100	-0.46730300
H	1.69677800	2.02644000	-2.91494200	H	7.73593700	-5.17183700	-0.81139600
H	1.47731900	-2.15692200	-2.29440200	H	8.96109900	-3.95403700	-1.07409300
				H	8.44228100	-4.33519800	0.55028700
				C	-3.74963000	5.46256200	4.43430100
				H	-3.61470100	6.30769900	3.79208800
				H	-4.79534300	5.27862600	4.56678800
				H	-3.29922100	5.66104100	5.38437400
				C	-5.84549400	-6.26055100	-0.86649700
				H	-5.16449200	-7.08585600	-0.86934300
				H	-6.39666600	-6.25609800	0.05061200
				H	-6.52300600	-6.35435000	-1.68934500

Table S9. Cartesian coordinates of complexes Eu-5 and Eu-6.

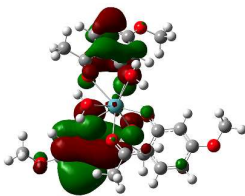
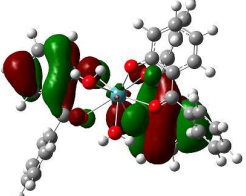
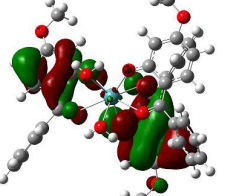
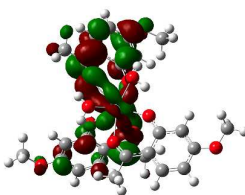
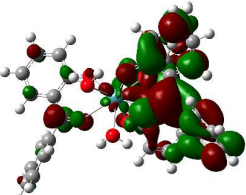
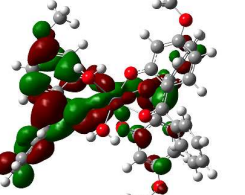
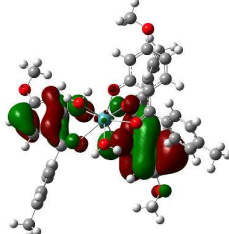
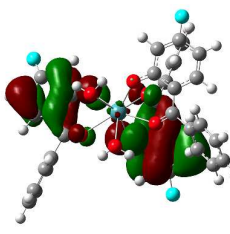
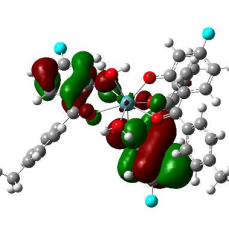
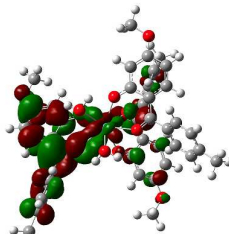
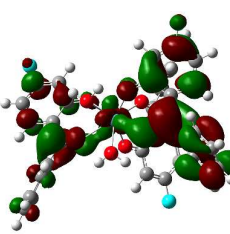
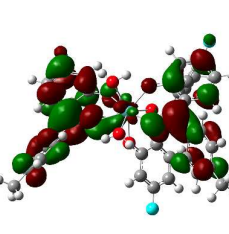
Eu-5				Eu-6			
Eu	0.33759000	-0.24815900	-0.87896300	Eu	0.34857000	-0.16462600	-0.98474100

O	1.81153800	1.47529100	-0.92652300	O	1.78845400	1.57986700	-1.01037300
O	2.68047000	-1.09851200	-0.95710400	O	2.72441600	-0.95970600	-0.98300400
O	0.64487300	-0.83118400	1.29521100	O	0.59490400	-0.83656500	1.18820500
O	-0.89953800	1.25912500	0.51756600	O	-0.87070000	1.30263400	0.40698400
O	-1.31374500	0.45346300	-2.37095500	O	-1.32043200	0.45555100	-2.49938800
O	-1.74442100	-1.54403100	-0.55144300	O	-1.67925200	-1.50682800	-0.64223800
C	3.06268200	1.77498200	-0.89583200	C	3.05710900	1.92061000	-1.05853300
C	3.44392200	3.14470500	-0.96677600	C	3.38850100	3.29637700	-1.22858700
H	2.66988500	3.89817900	-1.02958100	H	2.58558700	4.01772300	-1.30012000
C	4.76866800	3.49133600	-0.95653000	C	4.70542300	3.68105300	-1.29977100
C	5.81315500	2.55962400	-0.88299600	C	5.78115200	2.78085700	-1.21849000
H	6.84229500	2.89161000	-0.90470500	H	6.79806400	3.13832100	-1.31189600
C	5.46884900	1.23015800	-0.79637800	C	5.48203800	1.44412900	-1.03283700
H	6.25916700	0.49256400	-0.76212800	H	6.29336800	0.72818200	-0.99477400
C	4.11989200	0.78957100	-0.78525100	C	4.14329800	0.96881000	-0.93173500
C	3.81514900	-0.62519500	-0.72462000	C	3.87727100	-0.44482700	-0.75982700
C	4.87896800	-1.63087600	-0.38590800	C	4.94130000	-1.39625400	-0.32145000
C	5.67171600	-1.51151500	0.76146900	C	5.82273300	-1.10453900	0.73586400
H	5.55976200	-0.64748600	1.40562300	H	5.76576500	-0.14326200	1.23440200
C	6.57970400	-2.51482100	1.09451800	C	6.74047500	-2.06090700	1.17715800
H	7.17515700	-2.42283500	1.99575100	H	7.39796000	-1.82557400	2.00897500
C	6.72048100	-3.63290900	0.27459000	C	6.82061200	-3.32587300	0.57095000
H	7.43489700	-4.40736900	0.53001100	C	5.93260500	-3.61391400	-0.48217000
C	5.93583600	-3.75619100	-0.87240200	H	5.97249700	-4.58778100	-0.96182000
H	6.04306600	-4.62383500	-1.51362800	C	4.99986700	-2.67212000	-0.91346500
C	5.00851300	-2.76928600	-1.19166300	H	4.31367200	-2.91053600	-1.71931900
H	4.38524500	-2.86796700	-2.07305000	C	-0.02687900	-0.68247700	2.33647700
C	0.06293800	-0.67889000	2.43605500	C	0.14677500	-1.66957400	3.35098700
C	0.29923200	-1.63081800	3.46666100	H	0.79283800	-2.51382500	3.15019700
H	0.97226200	-2.45602600	3.27375200	C	-0.50402900	-1.54189000	4.55501800
C	-0.33072700	-1.50576900	4.67769100	C	-1.35500100	-0.46972100	4.86592700
C	-1.21433400	-0.46564000	4.98665400	H	-1.86564500	-0.43727200	5.81924900
H	-1.70357500	-0.43215300	5.95068500	C	-1.51602800	0.51427100	3.90608200
C	-1.43009500	0.48797600	4.01456300	H	-2.18905300	1.33805900	4.10977700
H	-2.12357700	1.29211700	4.22214600	C	-0.86756000	0.45854100	2.64192000
C	-0.81275900	0.43075500	2.74193300	C	-1.07954800	1.50180600	1.65536300
C	-1.09276700	1.44410500	1.73762100	C	-1.55343300	2.86336800	2.02704100
C	-1.64150100	2.78435800	2.12115600	C	-1.15491400	3.51244400	3.21027600
C	-1.16917600	3.49514300	3.23224000	H	-0.49762200	3.00697000	3.90860200
H	-0.40676900	3.05961400	3.86643100	C	-1.56133200	4.82386200	3.47054100
C	-1.64904200	4.77443100	3.50344400	H	-1.22906700	5.31544600	4.38017600
H	-1.26343000	5.32427900	4.35448200	C	-2.38121600	5.52230400	2.56976300
C	-2.61709900	5.34734300	2.68054400	C	-2.76774600	4.87182000	1.38157500

H	-2.99603400	6.33970900	2.89812100	H	-3.39287400	5.39706500	0.66495900
C	-3.09000500	4.64642000	1.57035900	C	-2.35186300	3.57213600	1.10649700
H	-3.83872700	5.09158600	0.92499100	H	-2.63229600	3.08770400	0.17829200
C	-2.59339200	3.38010400	1.28227700	C	-2.63602000	0.58879000	-2.42785000
H	-2.93564000	2.83988200	0.40826900	C	-3.25688000	1.65706000	-3.13008600
C	-2.59457700	0.62542900	-2.29419200	H	-2.63979200	2.33673800	-3.70240400
C	-3.18778200	1.72445200	-2.97091700	C	-4.62069600	1.82835300	-3.05420800
H	-2.55490900	2.40082400	-3.53049000	C	-5.46353300	0.99015600	-2.31094100
C	-4.53979900	1.93833000	-2.88551400	H	-6.52606600	1.18851300	-2.26334600
C	-5.40841300	1.11390300	-2.16239700	C	-4.87881600	-0.07413100	-1.64530500
H	-6.46378600	1.34466400	-2.10952300	H	-5.50418900	-0.72425100	-1.04611000
C	-4.85804200	0.02041500	-1.52855600	C	-3.47964200	-0.31981600	-1.68579500
H	-5.50576700	-0.62500900	-0.94995700	C	-2.91155400	-1.45800000	-0.97986600
C	-3.47223700	-0.26611200	-1.57222200	C	-3.74092300	-2.63948200	-0.60699400
C	-2.94333600	-1.43201400	-0.88243400	C	-3.45258300	-3.31086200	0.59844200
C	-3.83423900	-2.58728600	-0.53653800	H	-2.67274200	-2.91950800	1.24256900
C	-3.65742300	-3.22159600	0.70093500	C	-4.16529200	-4.45019900	0.96363700
H	-2.92318100	-2.82900900	1.39419200	H	-3.94060400	-4.94324700	1.90524100
C	-4.42345200	-4.33264900	1.03714000	C	-5.17170800	-4.97581600	0.13003300
H	-4.29422300	-4.80430600	2.00466500	C	-5.43636800	-4.31996000	-1.08325800
C	-5.35180100	-4.84275800	0.12854900	H	-6.19170300	-4.72121400	-1.75250600
H	-5.94153400	-5.71513700	0.38695300	C	-4.73917700	-3.16501400	-1.44775200
C	-5.51580500	-4.23313300	-1.11398300	H	-4.94895300	-2.68968000	-2.39942700
H	-6.22348400	-4.63697200	-1.82907700	O	0.73372100	-2.57712600	-1.23710300
C	-4.76906600	-3.10402100	-1.44286700	H	0.11091600	-3.05080000	-0.65623400
H	-4.89315600	-2.63860600	-2.41319700	O	0.98174100	0.03220300	-3.41954900
O	0.59861900	-2.72598100	-1.28393500	H	0.07122300	0.36537600	-3.62642100
H	-0.01372000	-3.21335800	-0.72020600	H	1.66854300	0.68680000	-3.63441800
O	0.97987200	-0.21515200	-3.40085000	H	1.66582100	-2.62130900	-0.93190900
H	0.13317300	0.20126700	-3.64020700	F	5.00222200	5.02874600	-1.47629000
H	1.67740500	0.40160400	-3.64604300	F	-5.19842200	2.89619400	-3.73363300
H	1.50252100	-2.90547700	-0.98865800	F	-0.32925000	-2.53247900	5.51885400
F	5.09948700	4.80179000	-1.03120800	C	7.84091900	-4.34429500	1.02547000
F	-5.06876900	3.01058000	-3.52185900	H	8.75299700	-4.29057800	0.41488500
F	-0.09959200	-2.44291300	5.62982400	H	8.13555900	-4.17872900	2.06696700
				H	7.45375300	-5.36554500	0.93993500
				C	-5.94677600	-6.20684900	0.53992900
				H	-5.27784500	-7.00388200	0.88587100
				H	-6.63590400	-5.98405600	1.36564700
				H	-6.54149700	-6.60076400	-0.29006300
				C	-2.83722600	6.93409500	2.85843300
				H	-2.62343000	7.60259800	2.01545700
				H	-3.92065100	6.97380100	3.03341400

				H	-2.34229100	7.34161200	3.74541200
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Table S10. Presentation of the energy levels, energy gaps and orbital composition distribution of the HOMO and LUMO for the complexes.

	Eu-1	Eu-2	Eu-3
HOMO			
E / eV	-5.58	-5.61	-5.56
contribution (Eu) / %	0.29	0.19	0.22
LUMO			
E/eV	-1.75	-2.12	-1.90
contribution (Eu) / %	22.10	0.37	3.26
HLG/eV	3.83	3.49	3.66
	Eu-4	Eu-5	Eu-6
HOMO			
E / eV	-5.49	-5.93	-5.84
% contribution (Eu)	0.23	0.22	0.35
LUMO			
E/eV	-1.81	-2.22	-2.12
%contribution (Eu)	4.65	0.61	0.82
HLG/eV	3.68	3.71	3.72

